

```
1 2 3 4 5 6
chain bonds :
   1-7 4-12 4-13 5-15 5-16 6-17 6-18 7-8
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
   4-12 4-13 5-15 5-16 6-17 6-18 7-8
exact bonds :
   1-2 1-6 1-7 2-3 3-4 4-5 5-6
isolated ring systems :
   containing 1 :
G1:H,Cl,Br,F,I,Hy,[*1],[*2]
Match level :
   1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 12:CLASS 13:CLASS
   15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 20:CLASS
Generic attributes :
   8:
   Saturation
                        : Unsaturated
   19:
   Saturation
                        : Unsaturated
   20:
```

: Saturated

ring nodes :

Saturation

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1839

L1 SCREEN CREATED

=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L2 SCREEN CREATED

=>

Uploading C:\STNEXP4\QUERIES\10009477 (rce).str

L3 STRUCTURE UPLOADED

=> que L3 AND L1 NOT L2

L4 QUE L3 AND L1 NOT L2

=> d 14

L4 HAS NO ANSWERS

L1 SCR 1839

L2 SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L3 STR

Ak²

Cb 1

G1 H, Cl, Br, F, I, Hy, [@1], [@2]

10/009,477 (RCE)

Structure attributes must be viewed using STN Express query preparation. L4 $\,$ QUE $\,$ L3 AND L1 NOT L2 $\,$

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1839

L5 SCREEN CREATED

=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L6 SCREEN CREATED

=>

Uploading C:\STNEXP4\QUERIES\10009477 (rce).str

L7 STRUCTURE UPLOADED

=> que L7 AND L5 NOT L6

L8 QUE L7 AND L5 NOT L6

=> d 18

L8 HAS NO ANSWERS

L5 SCR 1839

L6 SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L7 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation. L8 QUE L7 AND L5 NOT L6

=> s 18 sss sam

SAMPLE SEARCH INITIATED 08:28:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 8720 TO ITERATE

11.5% PROCESSED 1000 ITERATIONS

1 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 168806 TO 179994

PROJECTED ANSWERS: 1 TO 351

L9 1 SEA SSS SAM L7 AND L5 NOT L6

=> s 18 sss ful

FULL SEARCH INITIATED 08:29:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 174632 TO ITERATE

100.0% PROCESSED 174632 ITERATIONS

71 ANSWERS

10/009,477 (RCE)

SEARCH TIME: 00.00.05

L10 71 SEA SSS FUL L7 AND L5 NOT L6

=> s 110

L11 34 L10

=> d 111 1-34 bib,ab,hitstr

```
L11
     ANSWER 1 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
AN
     2003:591156 CAPLUS
DN
     139:149640
     Preparation of substituted quinazolin-4-ylamine analogs as VR1 capsaicin
ΤI
     receptor antagonists for relieving pain
IN
     Bakthavatchatam, Rajagopal; Blum, Charles A.; Brielmann, Harry L.;
     Caldwell, Timothy M.; De Lombaert, Stephane
PA
     Neurogen Corporation, USA
SO
     PCT Int. Appl., 294 pp.
     CODEN: PIXXD2
DT
     Patent
LА
     English
FAN.CNT 1
     PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO.
                                                            DATE
                            ,/-----
     ______
                      ____
                                           ______
                                                            _____
                           V20030731
PI
     WO 2003062209
                       A2
                                           WO 2003-US1563
                                                            20030117
     WO 2003062209
                       Α3
                            20030904
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, BE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD,
             RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
            NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRAI US 2002-349920P
                            20020117
                      Ρ
     US 2002-350527P
                            20020122
                       Ρ
OS
     MARPAT 139:149640
AΒ
     Substituted quinazolin-4-ylamine analogs (shown as I; variables defined
     below; e.g. (4-trifluoromethylphenyl)[7-(2-trifluoromethylphenyl)quinazoli
     n-4-yl]amine) are provided. Such compds. are ligands that may be used to
     modulate VR1 capsaicin receptor activity in vivo or in vitro (no data),
     and are particularly useful in the treatment of conditions assocd. with
     pathol. receptor activation in humans, domesticated companion animals and
     livestock animals. Pharmaceutical compns. and methods for using them to
     treat such disorders are provided, as are methods for using such ligands
     for receptor localization studies. For I; V, X, W, Y and Z are each
     independently N or CR1, with the proviso that at least one of V and X is
     N; U is N or CR2, with the proviso that if V and X are N, then U is CR2;
     R1 = H, halogen, hydroxy, amino, C1-C8 alkyl, haloC1-C8alkyl, C1-C8alkoxy,
     haloC1-C8alkoxy and mono- and di(C1-C8alkyl)amino. R2 = (i) H, halogen,
     cyano, or -COOH; (ii) C1-C8alkanoyl, C2-C8alkanone, or C1-C8carbamate,
     each of which is (un)substituted with 1-9 substituents = Rb, or (iii)
     -Rc-M-A-Ry, wherein: Rc is C0-C3alkyl; M is a bond, N(Rz), O, S, SO2,
     (C:0)pN(Rz), N(Rz)(C:0)p, SO2N(Rz), or N(Rz)SO2, wherein p is 0 or 1; A is
     a bond or C1-C8alkyl, (un) substituted with 1-3 Rb. Ry and Rz, if present,
     are: (a) independently H, C1-C8alkyl, C2-C8alkenyl, C2-C8alkynyl,
     C6-C10arylC1-C8alkyl, C2-C8alkyl ether, C1-C8alkoxy, a 4- to 10-membered
     carbocycle or heterocycle, or joined to R1 to form a 4- to 10-membered
     carbocycle or heterocycle, wherein each Ry and Rz = (un)substituted with
     1-9 Rb; or (b) joined to form a 4- to 10-membered carbocycle or
     heterocycle that is (un)substituted with 1-9 Rb; Ar2 is a 5- to 7-membered
     arom. heterocycle, (un) substituted with 1-3 LRa. Ar1 is a 5- to
     10-membered arom. carbocycle or heterocycle, (un) substituted with 1-3 LRa;
     L = bond, -O-, -C(O)-, -OC(O)-, -C(O)O-, -O-C(O)O-, -S(O)m-, -NRx-,
```

-C(O)NHRx-, -NHRxC(O)-, -NRxS(O)m-, -S(O)mNRx- and -N[S(O)mRx]S(O)m-; wherein m = 0, 1 and 2; and Rx = H and C1-C8alkyl; Ra = (i) H, halogen, cyano and nitro; and (ii) C1-C8alkyl, C2-C8alkenyl, C2-C8alkynyl, C2-C8alkyl ether, 3- to 10-membered heterocycles, mono- and di(C1-C8alkyl)amino and (3- to 10-membered heterocycle)C1-C6 alkyl, each of which is (un)substituted with 1-9 Rb. Rb = hydroxy, halogen, amino, aminocarbonyl, amido, cyano, nitro, C1-C8alkyl, C1-C8alkoxy, C1-C8alkylthio, C1-C8alkyl ether, hydroxyC1-C8alkyl, haloC1-C8alkyl, Ph, phenyl(C1-C8alkyl), mono and di(C1-C6 alkyl)amino, (SO2)C1-C8alkyl, 5- to 7-membered heterocycle and (5- to 7-membered heterocycle)(C1-C8alkyl). Although the methods of prepn. are not claimed, many example prepns. and characterization data for >500 examples of I are included.

IT 573683-86-OP, [2-[(5,6-Dihydro-4H-pyrimidin-1-yl)methyl]-7-(3trifluoromethylpyridin-2-yl)quinazolin-4-yl](4-trifluoromethylphenyl)amine
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); PAC
(Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic
use); ANST (Analytical study); BIOL (Biological study); PREP
(Preparation); USES (Uses)

(drug candidate and receptor detector; prepn. of substituted quinazolin-4-ylamine analogs as VR1 capsaicin receptor antagonists for relieving pain and for detecting receptors)

RN 573683-86-0 CAPLUS

CN

4-Quinazolinamine, 2-[(5,6-dihydro-1(4H)-pyrimidinyl)methyl]-N-[4-(trifluoromethyl)phenyl]-7-[3-(trifluoromethyl)-2-pyridinyl]- (9CI) (CA INDEX NAME)

```
L11 ANSWER 2 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
AN
     2003:221691 CAPLUS
DN
     138:255245
ΤI
     Preparation of imidazo[1,2-a]pyrimidines and intermediates and fungicide
     compositions containing the same
IN
     Ikegami, Hiroshi
     Sumitomo Chemical Company, Limited, Japan
PΑ
SO
     PCT Int. Appl., 98 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     Japanese
FAN.CNT 1
                      KIND
     PATENT NO.
                            DATE
                                           APPLICATION NO.
                                                            DATE
     _____
    WO 2003022850
PΤ
                       A1
                            20030320
                                           WO 2002-JP8718
                                                            20020829
        W: US
                             CY, CZ,
        RW: AT, BE, BG, CH,
                                     DE, DK, EE, ES, FI, FR, GB, GR, IE, IT,
             LU, MC, NL, PT, SE, SK, TR
                                           JP 2002-253211
     JP 2003155287
                       A2
                            ⁄20030527
                                                            20020830
PRAI JP 2001-266881
                            20010904
                       Α
OS
    MARPAT 138:255245
    Imidazo[1,2-a]pyrimidines représented by the general formula (I) have
AΒ
     excellent control activity against plant diseases: wherein R1 and R2 are
     each C1-C6 alkyl which may be substituted with one or more members
     selected from the group consisting of C1-C4 alkoxy, C2-C8 dialkylamino,
    C1-C4 alkylthio, C2-C5 alkoxycarbonyl, cyano and halogen, or the like, or
    R1 and R2 together with the nitrogen atom to which they are bonded may
     form a group derived from a 3- to 8-membered heterocycle; R3 is halogeno
    or C1-C4 alkyl; and Ar is Ph which may be substituted with a halogen atom
    or the like. Thus, reaction of di-Et malonate and 1-bromo-2,4,6-
     trifluorobenzene in presence of catalyst formed di-Et (2,4,6-
     trifluorophenyl) malonate (II). Reaction of II with 2-aminoimidazole
    hydrochloric acid salt formed 5,7-dihydroxy-6-(2,4,6-
    trifluorophenyl)imidazo-[1,2-a]pyrimidine, which underwent chlorine
    substitution reaction to give 5,7-dichloro-6-(2,4,6-
    trifluorophenyl)imidazo-[1,2-a]pyrimidine (III). Reaction of III with
     4-methylpiperidine gave 5-(4-methylpiperidin-1-yl)-6-(2,4,6-
    trifluorophenyl)-7-chloroimidazo-[1,2-a]pyrimidine (IV). III was tested
    to be an effective plant leaf fungicide.
    502500-62-1P 502501-73-7P 502502-33-2P
    502503-75-5P 502504-33-8P 502504-94-1P
    RL: AGR (Agricultural use); BUU (Biological use, unclassified); SPN
     (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (prepn. of imidazo[1,2-a]pyrimidine derivs. and intermediates for
       fungicide compns.)
RN
    502500-62-1 CAPLUS
CN
    Imidazo[1,2-a]pyrimidine, 7-chloro-5-(5,6-dihydro-1(4H)-pyrimidinyl)-6-
     (2,4,6-trifluorophenyl) - (9CI) (CA INDEX NAME)
```

RN 502501-73-7 CAPLUS

CN Imidazo[1,2-a]pyrimidine, 7-chloro-6-(2-chloro-6-fluorophenyl)-5-(5,6-dihydro-1(4H)-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 502502-33-2 CAPLUS

CN Imidazo[1,2-a]pyrimidine, 7-chloro-6-(2,6-difluorophenyl)-5-(5,6-dihydro-1(4H)-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 502503-75-5 CAPLUS

CN Imidazo[1,2-a]pyrimidine, 5-(5,6-dihydro-1(4H)-pyrimidinyl)-7-methyl-6-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

RN 502504-33-8 CAPLUS

CN Imidazo[1,2-a]pyrimidine, 6-(2-chloro-6-fluorophenyl)-5-(5,6-dihydro-1(4H)-pyrimidinyl)-7-methyl- (9CI) (CA INDEX NAME)

RN 502504-94-1 CAPLUS

CN Imidazo[1,2-a]pyrimidine, 6-(2,6-difluorophenyl)-5-(5,6-dihydro-1(4H)-pyrimidinyl)-7-methyl- (9CI) (CA INDEX NAME)

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L11
    ANSWER 3 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
AN
     2002:777929 CAPLUS
DN
     137:294954
     Preparation of 2-(4-substituted-2-oxo-1,2-dihydropyridin-3-yl)-
ΤI
     benzimidazoles as novel tyrosine kinase inhibitors
IN
     Wittman, Mark D.; Balasubramanian, Neelakantan; Velaparthi, Upender;
     Zimmermann, Kurt; Saulnier, Mark G.; Liu, Peiying; Sang, Xiaopeng;
     Frennesson, David B.; Stoffan, Karen M.; Tarrant, James G.
PA
     Bristol-Myers Squibb Company, USA
SO
     PCT Int. Appl., 249 pp.
     CODEN: PIXXD2
ידת
     Patent
     English
LΑ
FAN.CNT 1
                            DÁTE
     PATENT NO.
                      KIND
                                           APPLICATION NO. DATE
     ______
                            _____
                                           _____
PΙ
     WO 2002079192
                            20021010
                                           WO 2002-US9402
                                                           20020326
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, \overline{\text{IL}}, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                            20010328
PRAI US 2001-279327P
                       Ρ
    MARPAT 137:294954
os
     The title compds. [I; X = N, C, a bond, etc.; Y = O, S; W = N, C, O, S (if
AΒ
    W = O or S, then R9 is absent); R1-R9 = H, alkyl, cycloalkyl, etc.] and
     their pharmaceutically acceptable salts which inhibit tyrosine kinase
     enzymes thereby making them useful as anti-cancer agents, were prepd.
     Thus, reacting 3-[6-(imidazol-1-yl)-4-methyl-1H-benzimidazol-2-yl]-4-iodo-
     1H-pyridin-2-one (prepn. given) with (S)-(-)-2-phenylglycinol in the
    presence of N-methylmorpholine in DMF afforded 52% (S)-II which showed
     IC50 of 1.0 .mu.M in cytotoxicity assay (HT-29 human colon tumor cell
    line). 30 Of the exemplified compds. I showed kinase activity of <25.mu.M
    against one or more of the following kinases CDK, EMT, FAK, Her1, Her2,
     IGF, IR, LCK, MET, PDGF, VEGF. The compds. I are also useful for the
    treatment of other diseases which can be treated by inhibiting tyrosine
    kinase enzymes.
IT
     468740-83-2P 468740-84-3P
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (prepn. of 2-(4-substituted-2-oxo-1,2-dihydropyridin-3-yl)-
       benzimidazoles as novel tyrosine kinase inhibitors)
RN
     468740-83-2 CAPLUS
CN
    2(1H) -Pyridinone, 4-[(2S)-2-(3-chlorophenyl)-2-hydroxyethyl] amino]-3-[6-
     (5,6-dihydro-1(4H)-pyrimidinyl)-4-methyl-1H-benzimidazol-2-yl]- (9CI)
    INDEX NAME)
```

Absolute stereochemistry.

RN 468740-84-3 CAPLUS

CN 2(1H)-Pyridinone, 4-[[(2S)-2-(3-chloro-4-methoxyphenyl)-2-hydroxyethyl]amino]-3-[6-(5,6-dihydro-1(4H)-pyrimidinyl)-4-methyl-1H-benzimidazol-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2002:728879 CAPLUS

DN 137:263038

TI Preparation of triazoles as pharmaceuticals for treatment of autoimmune disease and inflammation

IN Tsuboi, Katsunori; Nakatsuka, Masashi; Kanai, Toshio; Fukuda, Nobuhisa

PA Sumitomo Pharmaceutical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 80 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO. KIND DATE

PI JP 2002275165 A2 20020925 JP 2001-300485 20010928 PRAI JP 2001-4881 A 20010112

OS MARPAT 137:263038

The compds. I [M = single-bond, O, S, SO, SO2, CQ, etc.; CQ = 1,3-dioxane ring, 1,3-dioxolane ring; Y1Y2 = H, halo, alkyl, haloalkyl, NO2, cyano, etc.; O-3 Y1 and Y2 exists resp.; R8, R9 = H, alkyl; R8R9 = hydrocarbon ring; R7 = H, R28, COR28, SO2R28, CO2R28, etc.; R7 is connected with N in triazole ring; R28 = alkyl, alkenyl, alkynyl, aryl, etc.; L = N:C(NR2R3)NR1R4, NR1C(:NR4)NR2R3, NR5R6; R1-R4 = H, OH, NO2, cyano, R29, OR29, COR29, etc.; R29 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl; R5, R6 = H, OH, R29, OR29, COR29, etc.] or their pharmaceutically acceptable salts are prepd. 4,3-PhFC6H3CHMeCO2Et (20 g) was treated with aminoguanidine hydrochloride in the presence of NaOMe in EtoH under reflux for 13 h to give 4.0 g 3-[1-(2-fluoro-1,1'-biphenyl-4-yl)ethyl]-1H-1,2,4-triazole-5-amine showing good inhibitory activity against adjuvant arthritis in rats.

IT 321879-37-2P 462646-02-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of triazoles as pharmaceuticals for treatment of autoimmune disease and inflammation)

RN 321879-37-2 CAPLUS

CN Methanone, [3-[1-[5-[5,6-dihydro-2-(4-morpholinyl)-1(4H)-pyrimidinyl]-1H-1,2,4-triazol-3-yl]ethyl]phenyl]phenyl- (9CI) (CA INDEX NAME)

RN 462646-02-2 CAPLUS

CN Morpholine, 4-[1-[5-(1-[1,1'-biphenyl]-4-ylethyl)-1H-1,2,4-triazol-3-yl]-1,4,5,6-tetrahydro-2-pyrimidinyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 462646-01-1 CMF C24 H28 N6 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

```
ANSWER 5 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
L11
ΑN
     2002:615577 CAPLUS
DN
     137:169536
TI
     Preparation of aryl-substituted tetrahydropyrimidines and related
     compounds as melanocortin-4 receptor binding compounds
IN
     Maguire, Martin P.; Dai, Mingshi; Vos, Tricia J.
PA
     Millennium Pharmaceuticals, Inc., USA
SO
     PCT Int. Appl., 228 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
                            DATE
     PATENT NO.
                      KIND
                                           APPLICATION NO. DATE
                                           _____
PΙ
     WO 2002062766
                      A2
                            20020815
                                           WO 2002-US3566
                                                            20020207
     WO 2002062766
                      A3
                            20021003
             AE, AG, AL, AM, AT, At, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1363890
                      A2
                            20031126
                                          EP 2002-718920 20020207
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
PRAI US 2001-778468
                            20010207
                      Α
    WO 2002-US3566
                       W
                            20020207
OS
    MARPAT 137:169536
AΒ
     Title compds. I [wherein A and B = independently (un) substituted biaryl,
     (hetero)aryl, Ph, (cyclo)alkyl, (cyclo)alkoxy, alkenyl, alkynyl, OH,
     acyl(oxy), carbamoyl, amino, thiol, amidino, imino, NO2, N3, etc.; L1 and
     L2 =- covalent bond or (un) substituted alkyl optionally interrupted by O,
     S, or N; r = covalent bond, CH, CH2, CHR1, CR1R2, or H; t = CH, CH2, CHR3,
     CR3R4, or H; s = CHR5, CR5R6, or absent; R = H, (un)substituted alkyl,
     arylalkyl, or heteroalkyl, and may optionally be linked to A, B, L1, or
    L2; R1-R6 = independently (un) substituted alkyl, halo, thiol, thioether,
     thioalkyl, alkoxy, and may be optionally linked to each other to form
     addnl. ring moieties, e.g., quinoxalinyl; or pharmaceutically acceptable
     salts thereof] were prepd. as melanocortin-4 receptor binding (MC4-R)
             For example, stirring a soln. of .alpha.-tolunitrile with
     diisopropylamine and BuLi in hexanes at -78.degree. under nitrogen for 1
    h, followed by addn. of HMPA and 1-chloromethylnaphthalene in THF,
    afforded 2-(2-naphthalen-1-ylethyl)benzonitrile. Heating the benzonitrile
    with 1,3-diaminopropane in the presence of H2S at 80.degree. for 72 h gave
    the tetrahydropyrimidinyl cycloaddn. product II. The latter exhibited
     exemplary inhibition of MC4-R in a scintillation proximity assay. I are
    useful for the treatment of disorders assocd. with pigmentation, bones, or
    wt. loss (no data).
IT
    326481-13-4P
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
```

Page 13

(MC4-R binding compd.; prepn. of aryl-substituted tetrahydropyrimidines and related compds. as melanocortin-4 receptor binding compds. for

(Uses)

treatment of pigmentation, bone, and wt. loss disorders)
RN 326481-13-4 CAPLUS

RN 326481-13-4 CAPLUS CN Pyrimidine, 1,4,5,6

Pyrimidine, 1,4,5,6-tetrahydro-1-(3-pyridinylmethyl)-2-[2-[(3-pyridinylmethyl)thio]phenyl]- (9CI) (CA INDEX NAME)

$$N - CH_2 - N$$

```
L11 ANSWER 6 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
AN
     2001:793434 CAPLUS
DN
     135:339275
ΤI
     Cyclic amidines, nicotinic acetylcholine .alpha.4.beta.2 receptor
     activators containing them, and pharmaceuticals
     Imoto, Masahiro; Iwanami, Tatsuya; Akabane, Minako; Tani, Yoshihiro
IN
PA
     Suntory, Ltd., Japan
SO
     Jpn. Kokai Tokkyo Koho, 25 pp.
                                                                    April pet
     CODEN: JKXXAF
DT
     Patent
LА
     Japanese
FAN.CNT 1
     PATENT NO.
                    KIND DATE
                                          APPLICATION NO.
                                                           DATE
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     JP 2001302643 A2
                           20011031
                                          JP 2000-120976
PT
                                                           20000421
    WO 2001081334
                     A2
                           20011101
                                          WO 2001-JP3378
                                                           20010420
    WO 2001081334
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                           20020808
        W: AU, CA, CN, KR, US
        RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
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    AU 2001048799
                                          AU 2001-48799
                      A5
                           20011107
                                                           20010420
     EP 1280793
                      A2
                           20030205
                                         EP 2001-921932
                                                           20010420
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, FI, CY, TR
     US 2003100769
                     A1
                           20030529
                                          US 2001-9477
                                                           20011211
PRAI JP 2000-120976
                      Α
                           20000421
    WO 2001-JP3378
                           20010420
                      W
    MARPAT 135:339275
OS
AΒ
    The activators, useful for treatment of brain function disorders, contain
     cyclic amidines I [A1, A2 = H, (un)substituted alkyl, (un)substituted
     aryl, (un)substituted heterocyclyl; X = (un)substituted C2H4,
     (un) substituted CH: CH, (un) substituted (CH2)3, (un) substituted CH2CH2NH]
     or their salts. Trimethylenediamine was cyclocondensed with Et
     (6-chloro-3-pyridyl)acetate and treated with fumaric acid to give I
     fumarate (A1 = H, A2 = 6-chloro-3-pyridylmethyl, X = CH:CH), which showed
     affinity with rat nicotinic acetylcholine .alpha.4.beta.2 receptor with Ki
    of 29 nM, vs. 1.6 nM, for nicotine. Pharmaceutical formulations contg. I
    are given.
IT
    371122-25-7P 371122-39-3P 371122-75-7P
    371122-81-5P 371122-83-7P 371122-85-9P
    371122-87-1P 371122-92-8P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of cyclic amidines as nicotinic acetylcholine .alpha.4.beta.2
        receptor activators)
RN
    371122-25-7 CAPLUS
CN
    Pyrimidine, 1-[(6-chloro-3-pyridinyl)methyl]-1,4,5,6-tetrahydro-,
     (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)
    CM
         371122-24-6
    CRN
    CMF C10 H12 C1 N3
```

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 371122-39-3 CAPLUS

CN Pyrimidine, 1,2-bis[(6-chloro-3-pyridinyl)methyl]-1,4,5,6-tetrahydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 371122-38-2 CMF C16 H16 C12 N4

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 371122-75-7 CAPLUS

CN Pyrimidine, 1-[(5,6-dichloro-3-pyridinyl)methyl]-1,4,5,6-tetrahydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 371122-74-6 CMF C10 H11 C12 N3

$$C1$$
 N
 CH_2
 N
 N

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 371122-81-5 CAPLUS

CN Pyrimidine, 1-[2-(6-chloro-3-pyridinyl)ethyl]-1,4,5,6-tetrahydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 371122-80-4 CMF C11 H14 C1 N3

$$C1$$
 N
 CH_2-CH_2
 N
 N

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 371122-83-7 CAPLUS
CN Pyridazine, 3-[(5,6-dihydro-1(4H)-pyrimidinyl)methyl]-,
(2E)-2-butenedioate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 371122-82-6

CMF C9 H12 N4

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 371122-85-9 CAPLUS

CN Pyrimidine, 1,4,5,6-tetrahydro-1-[(6-methyl-3-pyridinyl)methyl]-, (2E)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 371122-84-8 CMF C11 H15 N3

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 371122-87-1 CAPLUS

CN Pyrimidine, 1,4,5,6-tetrahydro-1-(3-pyridinylmethyl)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 371122-86-0

CMF C10 H13 N3

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 371122-92-8 CAPLUS

CN Pyrimidine, 1-[(2-chloro-5-thiazolyl)methyl]-1,4,5,6-tetrahydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 371122-91-7 CMF C8 H10 C1 N3 S

$$N - CH_2$$
 $N - CH_2$ $N - CH_2$

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

IT 371122-24-6 371122-38-2 371122-74-6

371122-80-4 371122-82-6 371122-84-8

371122-86-0 371122-91-7

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(prepn. of cyclic amidines as nicotinic acetylcholine .alpha.4.beta.2 receptor activators)

RN 371122-24-6 CAPLUS

CN Pyrimidine, 1-[(6-chloro-3-pyridinyl)methyl]-1,4,5,6-tetrahydro- (9CI)

(CA INDEX NAME)

RN 371122-38-2 CAPLUS

CN Pyrimidine, 1,2-bis[(6-chloro-3-pyridinyl)methyl]-1,4,5,6-tetrahydro-(9CI) (CA INDEX NAME)

RN 371122-74-6 CAPLUS

CN Pyrimidine, 1-[(5,6-dichloro-3-pyridinyl)methyl]-1,4,5,6-tetrahydro- (9CI) (CA INDEX NAME)

RN 371122-80-4 CAPLUS

CN Pyrimidine, 1-[2-(6-chloro-3-pyridinyl)ethyl]-1,4,5,6-tetrahydro- (9CI) (CA INDEX NAME)

RN 371122-82-6 CAPLUS

CN Pyridazine, 3-[(5,6-dihydro-1(4H)-pyrimidinyl)methyl]- (9CI) (CA INDEX NAME)

RN 371122-84-8 CAPLUS

CN Pyrimidine, 1,4,5,6-tetrahydro-1-[(6-methyl-3-pyridinyl)methyl]- (9CI) (CA INDEX NAME)

Me
$$N \subset H_2 \subset N \subset N$$

RN 371122-86-0 CAPLUS

CN Pyrimidine, 1,4,5,6-tetrahydro-1-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

RN 371122-91-7 CAPLUS

CN Pyrimidine, 1-[(2-chloro-5-thiazolyl)methyl]-1,4,5,6-tetrahydro- (9CI) (CA INDEX NAME)

$$N \longrightarrow CH_2 \longrightarrow S \longrightarrow C1$$

```
ANSWER 7 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
AN
     2001:185754 CAPLUS
DN
     134:237479
     Preparation of 5-amino-substituted triazolopyridines for treating diseases
ΤI
     related to the adenosine A2A receptor
     Huber Trottmann, Gerda; Hunkeler, Walter; Jakob-Roetne, Roland;
IN
     Kilpatrick, Gavin John; Nettekoven, Matthias Heinrich; Riemer, Claus
PA
     F. Hoffmann-La Roche A.-G., Switz.
     PCT Int. Appl., 698 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LΑ
FAN.CNT 1
     PATENT NO.
                     KIND DATE
                                          APPLICATION NO. DATE
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                            20010315
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PT
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            MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,
            TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ,
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            DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
            CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                         US 2000-645127
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                                                           20000824
    BR 2000013792
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                                          BR 2000-13792
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    EP 1214322
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                      A2
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            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL
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                      Α
                            20020305
                                          NO 2002-1077
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PRAI EP 1999-117578
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                      Α
    WO.2000-EP8372
                      W
                           20000828
OS
    MARPAT 134:237479
    The title compds. [I; R1 = (un) substituted 5-6 membered heteroaryl, contg.
AΒ
     1-3 heteroatoms selected from N, O, S (wherein the heteroaryl may be
    optionally linked to the pyrazole ring via an alkylene or alkenylene),
     (un) substituted Ph, O(CH2) nPh, etc.; R2, R4 = H, CN, SO2Ph; R3 = H, halo,
     (un) substituted 5-6 membered heteroaryl, contg. 1-3 heteroatoms, selected
     from N, O or S, etc.; R5 = NR2 (wherein R = H, alkyl, Ph, etc.); n = 0-4],
    useful for the treatment of diseases related to the adenosine A2A
    receptor, were prepd. and formulated. Thus, treating 5-bromo-2-
    methoxypyridine with acrylonitrile in the presence of Et3N and
     Pd(PPh3)2Cl2 in DMF followed by reaction of the resulting
     3-(6-methoxypyridin-3-yl)acrylonitrile with 3-benzenesulfonylmethyl-5-
     furan-2-yl-1H-[1,2,4]triazole (prepn. given) in the presence of NaH
     afforded I [R1 = 2-furyl; R2, R4 = H; R3 = 6-methoxypyridin-3-yl; R5 =
    NH2] which showed pKi of 7.9 in the human A2A binding assay.
IT
    329972-24-9P 329973-39-9P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of 5-amino-substituted triazolopyridines for treating diseases
        related to the adenosine A2A receptor)
RN
     329972-24-9 CAPLUS
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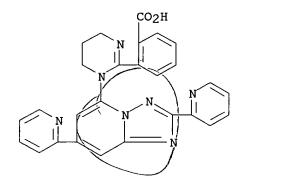
Benzoic acid, 2-[1,4,5,6-tetrahydro-1-[2-phenyl-7-(4

CN

pyridinyl)[1,2,4]triazolo[1,5-a]pyridin-5-yl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 329973-39-9 CAPLUS

CN Benzoic acid, 2-[1-(2,7-di-2-pyridinyl[1,2,4]triazolo[1,5-a]pyridin-5-yl)-1,4,5,6-tetrahydro-2-pyrimidinyl]- (9CI) (CA INDEX NAME)





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L11 ANSWER 9 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
AN
    2001:63983 CAPLUS
DN
     134:131527
     Preparation and effect of heteroaromatic ring compounds against autoimmune
ΤI
    disorders and chronic inflammation
IN
    Nakatsuka, Masashi; Nakatani, Shogo; Okada, Shin-ichiro; Tsuboi,
    Katsunori; Nishikaku, Fumio
    Sumitomo Pharmaceuticals Co., Ltd., Japan
PA
SO
    PCT Int. Appl., 190 pp.
    CODEN: PIXXD2
DΤ
    Patent
    Japanese
LА
FAN.CNT 1
                     KIND DATE
                                          APPLICATION NO.
                                                         DATE
    PATENT NO.
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                                                          -----
                                        WO 2000-JP4616 20000710
    WO 2001005774
                    A1
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           AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
            HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
            LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
            SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
            YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
            DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
            CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                      A1 20020502
                                        EP 2000-944389 20000710
    EP 1201661
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL
PRAI JP 1999-201447
                           19990715
                     Α
    JP 2000-58217
                           20000303
                      Α
    WO 2000-JP4616
                           20000710
os
    MARPAT 134:131527
AΒ
    Title compds. [I; R1 = F, C6H5CO, C6H5CHO2(CH2)2; R2 = H, C6H5; R3 = H,
    CH3; R4 = H, CH3; R5 = CH3, CH2CH2N[(CH2)2]O; R6 = H, CH3; R4-R5 =
    CH2CH2OCH2CH2, CH2CH2SCH2CH2, CH2CH2S(:O)(:O)CH2CH2; R6 = H, CH3; R7 =
    CH3, H, CH2CH2OH, CN, C(NH)N[(CH2)2]20; R5-R7 = CH2CH2, CH2CH2CH2,
    CH2CH0HCH2; R6-R7 = CH2CH2OCH2CH2; R8 = H, CH3; R9 = H, CH3; X = N, NCH3,
    S; Y = NCH3, S, NH, NSO2C6H5; Z = CH, O, S, N; dotted line = single,
    double bond] and pharmaceutically acceptable salts exhibiting excellent
    phys. properties and potent ameliorative effects against both immune
    disorders and chronic inflammation are prepd. Thus, the title compd. II
    was prepd. and tested.
IT
    321879-37-2P
    RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
    study); PREP (Preparation); USES (Uses)
        (prepn. and effect of heteroarom. ring compds. against immune disorders
       and chronic inflammation)
RN
    321879-37-2 CAPLUS
CN
    Methanone, [3-[1-[5-[5,6-dihydro-2-(4-morpholinyl)-1(4H)-pyrimidinyl]-1H-
```

1,2,4-triazol-3-yl]ethyl]phenyl]phenyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L11 ANSWER 10 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
     2000:769086 CAPLUS
ΑN
     133:335159
DN
     Preparation of N-pyridinyl-2-[(thienylcarbonyl)amino]benzamides and
ΤI
     analogs as anticoagulants
     Arnaiz, Damian O.; Chou, Yuo-ling; Griedel, Brian D.; Karanjawala, Rushad
IN
     E.; Kochanny, Monica J.; Lee, Wheeseong; Liang, Amy Mei; Morrissey,
     Michael M.; Phillips, Gary B.; Sacchi, Karna Lyn; Sakata, Steven T.; Shaw,
     Kenneth J.; Snider, R. Michael; Wu, Shung C.; Ye, Bin; Zhao, Zuchun
PA
     Berlex Laboratories, Inc., USA
SO
     U.S., 113 pp., Cont.-in-part of U.S. Ser. No. 994,284, abandoned.
                                                                   gove 2/2
     CODEN: USXXAM
DT
     Patent
     English
LΑ
FAN.CNT 2
     PATENT NO.
                     KIND DATE
                                          APPLICATION NO.
                                                           DATE
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PΙ
     US 6140351
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                                         US 1998-187459
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     WO 9932477
                           19990701
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             NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT,
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     AU 9918759
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     AU 751856
                      B2
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     EP 1040108
                      A1
                           20001004
                                          EP 1998-963519
                                                           19981127
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     JP 2001526283
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     NZ 503809
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                                          NZ 1998-503809
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                                        ZA 1998-11599
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                      Α
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                                          NO 2000-3111
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                      В1
                           20020430
                                          US 2000-631450
                                                           20000803
     US 6498185
                      В1
                           20021224
                                          US 2000-631452
                                                           20000803
PRAI US 1997-994284
                      В2
                           19971219
     US 1998-187459
                      Α
                           19981105
     WO 1998-EP7650
                      W
                           19981127
os
     MARPAT 133:335159
AB
     REZDR3 [I; D,E = Z1NR5C(:X), Z1NR5SO0-2, etc.; R,R3 = (un)substituted
     heterocyclyl or -aryl; R5 = H, (ar)alkyl, aryl; X = O, S, H2; Z =
     (un) substituted heterocyclylene or -arylene; Z1 = bond, alkylene,
     alkylidene, etc.] were prepd. as factor Xa, thrombin, and prothrombinase
     inhibitors. Thus, H2NZCONHC6H4Cl-4 (Z = 4-chloro-1,2-phenylene) (prepn.
     given) was N-acylated by 3-chloro-4-chloromethyl-2-thiophenecarbonyl
     chloride and the product aminated by 1-methylpiperazine to give title
     compd. II. Data for biol. activity of I were given.
```

IT 229336-18-9P 229340-52-7P 229343-43-5P

> RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of N-pyridinyl-2-[(thienylcarbonyl)amino]benzamides and analogs as anticoagulants)

RN 229336-18-9 CAPLUS CN 2-Thiophenecarboxamide, 3-chloro-N-[4-chloro-2-[[(5-chloro-2-pyridinyl)amino]carbonyl]-6-methoxyphenyl]-4-[(5,6-dihydro-1(4H)-pyrimidinyl)methyl]- (9CI) (CA INDEX NAME)

RN 229340-52-7 CAPLUS

CN 2-Thiophenecarboxamide, 3-chloro-N-[4-chloro-2-[[(5-chloro-2-pyridinyl)amino]carbonyl]-6-methoxyphenyl]-4-[(5,6-dihydro-1(4H)-pyrimidinyl)methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 229336-18-9

CMF C23 H20 C13 N5 O3 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 229343-43-5 CAPLUS

CN 2-Thiophenecarboxamide, 3-chloro-N-[4-chloro-2-[[(5-chloro-2-pyridinyl)amino]carbonyl]-6-methoxyphenyl]-4-[(5,6-dihydro-5-hydroxy-1(4H)-pyrimidinyl)methyl]-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 229343-42-4

CMF C23 H20 C13 N5 O4 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 11 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
L11
AN
     2000:688225 CAPLUS
DN
     133:252445
TI
     Preparation of fused pyridopyridazine inhibitors of cGMP phosphodiesterase
IN
     Yu, Guixue; Macor, John; Chung, Hyei-jha; Humora, Michael; Katipally,
     Kishta; Wang, Yizhe; Kim, Soojin
PA
     Bristol-Myers Squibb Company, USA
SO
     PCT Int. Appl., 137 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO.
                                                            DATE
     _____
                            ______
                                           -----
                                                            ______
     WO 2000056719
                            20000928
                                           WO 2000-US6100
PT
                       A1
                                                            20000309
         W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
             CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
             MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
             SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     EP 1165521
                      A1 20020102
                                         EP 2000-916180
                                                            20000309
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     AU 765128
                            20030911
                                           AU 2000-37327
                       В2
                                                            20000309
     US 6316438
                       В1
                            20011113
                                           US 2000-526162
                                                            20000315
PRAI US 1999-125488P
                       Ρ
                            19990322
     US 1999-148009P
                       Ρ
                            19990810
     WO 2000-US6100
                       W
                            20000309
os
     MARPAT 133:252445
AΒ
     The title compds. [I; Y = N, CR5; Z = N, CR6 (provided that at least one
     of Y and Z = N); R1, R2 = H, halo, SR7, etc.; R3 = H, alkyl, arylalkyl; R4
     = H, halo, alkyl, etc.; R5, R6 = H, halo, alkyl; R7 = H, alkyl,
     cycloalkyl, etc.] and their pharmaceutically acceptable salts, inhibitors
     of cGMP PDE, esp. type 5, useful in treating cardiovascular and sexual
     disorders, were prepd. E.g., a multi-step synthesis of I [Y = N; Z = CH;
     R1 = 4-hydroxypiperidin-1-y1; R2 = (3-C1-4-MeOC6H3)CH2NH; R3 = Et; R4 = H]
     was given. Compds. I are effective at 0.05-100 mg/kg/day.
IT
     296250-13-0P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of fused pyridopyridazine inhibitors of cGMP phosphodiesterase)
RN
     296250-13-0 CAPLUS
     Pyrimidine, 1-[[1-[9-[[(3-chloro-4-methoxyphenyl)methyl]amino]-3-ethyl-3H-
CN
     pyrazolo[4',3':5,6]pyrido[3,4-d]pyridazin-6-yl]-1H-imidazol-4-yl]carbonyl]-
     1,4,5,6-tetrahydro- (9CI) (CA INDEX NAME)
```

$$\begin{array}{c} \text{C1} \\ \text{CH}_2-\text{NH} \\ \text{N} \\ \text{N} \\ \text{Et} \\ \end{array}$$

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L11 ANSWER 15 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
- AN 1998:126254 CAPLUS
- DN 128:204878
- TI Preparation of pyrazinobenzothiazine derivatives and analogs for the treatment of inflammation and autoimmune diseases
- IN Kaneko, Toshihiko; Clark, Richard; Ohi, Norihito; Ozaki, Fumihiro; Kawahara, Tetsuya; Kamada, Atsushi; Okano, Kazuo; Yokohama, Hiromitsu; Muramoto, Kenzo; Arai, Tohru; Ohkuro, Masayoshi; Takenaka, Osamu; Sonoda, Jiro
- PA Eisai Co., Ltd., Japan; Kaneko, Toshihiko; Clark, Richard; Ohi, Norihito; Ozaki, Fumihiro; Kawahara, Tetsuya; Kamada, Atsushi; Okano, Kazuo; Yokohama, Hiromitsu; et al.
- SO PCT Int. Appl., 1344 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

	PA'	TENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO	9806720	A1	19980219	WO 1997-JP2787	19970808
		W: AU, CA,	CN, HU	, JP, KR, MX,	NO, NZ, RU, US	
		RW: AT, BE,	CH, DE	, DK, ES, FI,	FR, GB, GR, IE, IT,	, LU, MC, NL, PT, SE
	ΑU	9737849	A1	19980306	AU 1997-37849	19970808
	ZΑ	9707103	Α	19990208	ZA 1997-7103	19970808
	EΡ	934941	A1	19990811	EP 1997-934750	19970808
		R: AT, BE,	CH, DE	, DK, ES, FR,	GB, GR, IT, LI, LU,	, NL, SE, PT, IE, FI
	US	6518423	B1	20030211	US 1999-230852	19990405
PRAI	JΡ	1996-210344	Α	19960809	•	
	WO	1997-JP2787	W	19970808		

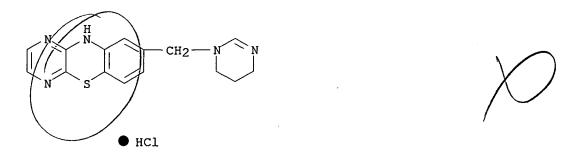
- OS MARPAT 128:204878
- AB The title compds. I [R1 to R3 are the same or different and each represents hydrogen, optionally substituted lower alkyl, optionally substituted cycloalkyl, etc., provided that when R1 to R3 are all optionally substituted lower alkyl groups, they do not simultaneously represent Me groups; R represents hydrogen, lower alkyl, etc.; E represents N, C, etc.; Z represents O, S, SO, SO2, etc.; and the ring G represents an optionally substituted heteroaryl ring having at least one nitrogen atom] are prepd. I are useful in the treatment and prevention of inflammatory immunol. diseases, autoimmune diseases, rheumatism, collagen disease, asthma, nephritis, ischemic reflow disorders, psoriasis, atopic dermatitis or rejection reactions following organ transplantation. compd. (syn)-[3-(10H-pyrazino[2,3-b][1,4]benzothiazin-8-ylmethyl)-3azabicyclo[3.3.1]nona-9-yl]acetic acid (II) at 10 mg/kg orally gave 65% inhibition of carrageenin-induced inflammation in rats. II in vitro showed IC50 of 2.3 .mu.M against the expression of ICAM-1.
- IT 203659-68-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrazinobenzothiazine derivs. and analogs for treatment of inflammation and autoimmune diseases)

RN 203659-68-1 CAPLUS

CN 1H-Pyrazino[2,3-b][1,4]benzothiazine, 8-[(5,6-dihydro-1(4H)-pyrimidinyl)methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/009,477 (RCE)

- L11 ANSWER 17 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
- 1996:577408 CAPLUS AΝ
- 125:276744 DN
- Synthesis and radical polymerization of novel vinyl monomers having a TISame on #16 imidazoline and pyrimidine moiety
- ΑU Seckin, Turgay; Alici, Bulent; Cetinkaya, Engin; Ozdemir, Ismail
- Fac. Art Sci. Chem., Inonu Univ., Malatya, TR-44069, Turk. CS
- SO Polymer Bulletin (Berlin) (1996), 37(4), 443-450 CODEN: POBUDR; ISSN: 0170-0839
- PB Springer
- DT Journal
- LΑ English
- Alkylation of the methylene-bridged tetrahydropyrimidine derivs. by AB chloromethylstyrene produces bridged bis(4-vinylbenzyl)-1,4,5,6tetrahydropyrimininum salts in high yields. Similar procedures are used to prep. 2-imidazolinium derivs. The quaternary salts which support functional side groups of potential biomedical interest are characterized by spectroscopic methods. These monomers are readily polymd. free radically in DMF soln. at moderate temps. The sol. and insol. polymers contg. 2-imidazolinium and 1,4,5,6-tetrahydropyrimidinum salts exhibited antibacterial activities against Escherichia coli.
- IT182947-47-3
 - RL: RCT (Reactant); RACT (Reactant or reagent) (prepn. and polymn. of vinyl monomers having a imidazoline or pyrimidine moiety)
- RN 182947-47-3 CAPLUS
- Pyrimidine, 1,1'-(1,2-ethanediyl)bis[1,4,5,6-tetrahydro- (9CI) (CA INDEX CN NAME)

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L11 ANSWER 18 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
AN
     1995:219295 CAPLUS
DN
     122:10060
TI
     Preparation of 1-(3-pyridyl)-2-(dihalonitromethyl)-1,3-diazacyclopent-2-
     enes and -diazacyclohex-2-enes as pesticides.
IN
     Munro, David; Patel, Bipin
PΑ
     Shell Internationale Research Maatschappij B.V., Neth.
SO
     PCT Int. Appl., 26 pp.
     CODEN: PIXXD2
DΤ
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                      KIND DATE
                                            APPLICATION NO.
                                                             DATE
                            _____
     _____
                                            _____
PΙ
                            19941013
                                           WO 1994-EP1089
     WO 9422851
                       A1
                                                              19940406
         W: AU, BR, CA, CN, HU, JP, KR, KZ, RU, UA
         RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
     AU 9465393
                       A1
                             19941024
                                            AU 1994-65393
                                                              19940406
     ZA 9402392
                       Α
                           19950116
                                            ZA 1994-2392
                                                              19940407
PRAI EP 1993-302748
                             19930407
     WO 1994-EP1089
                             19940406
     CASREACT 122:10060; MARPAT 122:10060
     Title compds. [I; n = 1, 2; R1 = (substituted) 3-pyridyl group; R2 = H, alkyl, haloalkyl; X, X1 = halo], were prepd. Thus, 2-nitromethylene-1-(6-
AB
     methoxy-3-pyridyl)hexahydropyrimidine was stirred with N-chlorosuccinimide
     in CCl4 for 24 h to give 1-(6-methoxy-3-pyridyl)-2-(dichloronitromethyl)-
     1,3-diazacyclohex-2-ene. I showed a toxicity index [[LC50
     (parathion)/LC50 (I)] .times. 100] = 1000-28000 against Nephotettix
     cincticeps.
IT
     159336-02-4P 159336-06-8P 159336-07-9P
     159336-09-1P
     RL: AGR (Agricultural use); BAC (Biological activity or effector, except
     adverse); BSU (Biological study, unclassified); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of 2-(dihalonitromethyl)-1,3-diazacyclopent-2-enes and
        -diazacyclohex-2-enes as pesticides)
RN
     159336-02-4, CAPLUS
     Pyrimidine, 2-(dichloronitromethyl)-1,4,5,6-tetrahydro-1-(6-methoxy-3-
CN
     pyridinyl) - (9CI) (CA INDEX NAME)
       CCl2-NC
RN
     159336-06-8 CAPLUS
     Pyrimidine, 1-(6-bromo-3-pyridinyl)-2-(dichloronitromethyl)-1,4,5,6-
CN
```

tetrahydro- (9CI) (CA INDEX NAME)

RN

159336-07-9 CAPLUS
Pyrimidine, 1-(6-chloro-3-pyridinyl)-2-(dichloronitromethyl)-1,4,5,6-CN tetrahydro- (9CI) (CA INDEX NAME)

RN 159336-09-1 CAPLUS

Pyrimidine, 1-(6-chloro-3-pyridinyl)-2-(difluoronitromethyl)-1,4,5,6-CN tetrahydro- (9CI) (CA INDEX NAME)

L11 ANSWER 20 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1994:106926 CAPLUS

DN 120:106926

TI Novel syntheses of tricyclic, N-aryl, pyridine- and pyrazine-fused pyrimidones

AU Friary, Richard; McPhail, Andrew T.; Seidl, Vera

CS Schering-Plough Res. Inst., Kenilworth, NJ, 07033-0539, USA

SO Collection of Czechoslovak Chemical Communications (1993), 58(5), 1133-50 CODEN: CCCCAK; ISSN: 0010-0765

DT Journal

LA English

OS CASREACT 120:106926

AB 2-Methylthio-2-imidazoline and 2-methylthio-1,4,5,6-tetrahydro-2pyrimidine amidated 2-chloro-3-pyridine- and 2-chloro-3-pyrazinecarbonyl chlorides. The products, (pyridinyl/pyrazinylcarbonyl)imidazoles and -pyrimidines I (X = CH, N, n = 1, 2), reacted with ArNH2 (Ar = Ph, N, n = 1, 2)substituted Ph) forming a series of tricyclic, linearly fused N-aryl pyrimidones II. Included among these pyrimidones were 10-aryl-2,3-dihydroimidazo[1,2-a]pyrido[2,3-d]pyrimidin-5(10H)-ones, 11-aryl-2,3,4,11-tetrahydropyrido[2,3-d]pyrimido[1,2-a]pyrimidin-6(6H)ones, 10-aryl-2,3-dihydroimidazo[1,2-a]pyrazino[2,3-d]pyrimidin-5(10H)ones, and 11-aryl-2,3,4,11-tetrahydropyrimido[1,2-a]pyrazino[2,3d]pyrimidin-6(6H)-ones. 4,5,6,7-Tetrahydro-2-(methylthio)1H-1,3-diazepine amidated the Et hydrogen carbonate of 2-(phenylamino)-3-pyridinecarboxylic acid, forming 12-phenyl-2,3,4,5-tetrahydropyrido[2',3':4,5]pyrimido[1,2a][1,3]diazepine-7(12H)-one. A single-crystal X-ray anal. and an unambiguous synthesis established the structure of the linearly fused isomer 10-phenyl-2,3-dihydroimidazo[1,2-a]pyrido[2,3-d]pyrimidin-5(10H)-

IT 108409-42-3P 108409-44-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and cyclocondensation of, with arylamines)

RN 108409-42-3 CAPLUS

CN Pyrimidine, 1-[(2-chloro-3-pyridinyl)carbonyl]-1,4,5,6-tetrahydro-2-(methylthio)- (9CI) (CA INDEX NAME)

RN 108409-44-5 CAPLUS

CN Pyrimidine, 1-[(3-chloropyrazinyl)carbonyl]-1,4,5,6-tetrahydro-2-(methylthio)- (9CI) (CA INDEX NAME)

- L11 ANSWER 21 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
- AN 1992:448211 CAPLUS
- DN 117:48211
- TI Preparation of 1-azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid compounds as antimicrobial agents
- IN Murata, Masayoshi; Chiba, Toshiyuki; Tsutsumi, Hideo; Yamada, Akira; Hattori, Kohji
- PA Fujisawa Pharmaceutical Co., Ltd., Japan
- SO PCT Int. Appl., 85 pp. CODEN: PIXXD2
- DT Patent
- LA English
- FAN. CNT 1

EMM.	CNII		
	PATENT NO.	KIND DATE	APPLICATION NO. DATE
ΡI	WO 9202521	A1 19920220	WO 1991-JP997 19910725
	W: CA, JP,	KR, US	
	RW: AT, BE,	CH, DE, DK, ES, FR	R, GB, GR, IT, LU, NL, SE
	JP 04234886	A2 19920824	JP 1991-196181 19910308
	JP 06503803	T2 19940428	JP 1991-512378 19910725
PRAI	GB 1990-16507	19900727	•
	JP 1991-196181	19910308	
	GB 1990-5265	19900308	
	WO 1991-JP997	19910725	

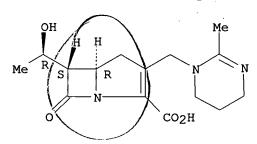
- OS MARPAT 117:48211
- AB The title compds. [I; R1 = (protected) carboxy; R2 = (protected) hydroxyalkyl; R3 = azetidinyl, pyrrolidinyl, imidazolidinyl, etc.; R10 = H, alkyl; A = alkylene] are prepd. A soln. of 5.14 g triester II in THF and EtOH was treated with Ph3P, dimedone, HOAc, and (Ph3P)4Pd with stirring at room temp., the ppt. was worked up and treated with MeC(:NH)OEt.HCl at pH 8.5 to give 0.49 g III. One I showed MIC of .ltoreq.0.025 .mu.g/mL against Staphylococcus epidermidis 89.
- IT 142255-21-8P 142255-23-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of, as antimicrobial agent)

- RN 142255-21-8 CAPLUS
- CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(5,6-dihydro-2-methyl-1(4H)-pyrimidinyl)methyl]-6-(1-hydroxyethyl)-7-oxo-, [5R-[5.alpha.,6.alpha.(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





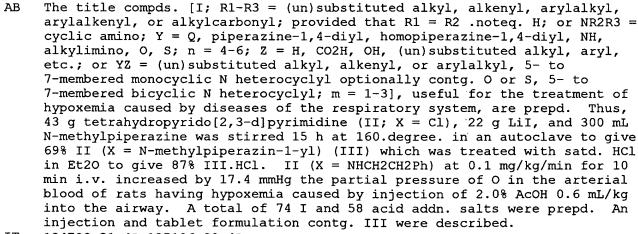
RN 142255-23-0 CAPLUS

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(5,6-dihydro-1(4H)-pyrimidinyl)methyl]-6-(1-hydroxyethyl)-7-oxo-, [5R-[5.alpha.,6.alpha.(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

- L11 ANSWER 22 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
- AN 1991:471646 CAPLUS
- DN 115:71646
- TI Preparation of bicyclic pyrimidine derivatives and pharmaceutical compositions containing them for treatment of hypoxemia
- IN Sakuma, Yasuji; Hasegawa, Masaichi; Kataoka, Kenichiro; Hoshina, Kenji; Yamazaki, Noboru; Kadota, Takashi; Yamaguchi, Hisao
- PA Teijin Ltd., Japan
- SO PCT Int. Appl., 83 pp. CODEN: PIXXD2
- DT Patent
- LA Japanese
- FAN. CNT 1

ran.	PATENT NO.	KIND DATE	APPLICATION NO.	DATE
PI			002 WO 1990-JP1313	19901011
	•	HU, JP, KR, T	JS ES, FR, GB, GR, IT, NL, SE	
			CA 1990-2067221	
	CA 2067221	C 199704	115	
	AU 9065220	A1 19910!	316 AU 1990-65220	19901011
	AU 645504	B2 19940:	.20	
	EP 495982	A1 19920	729 EP 1990-914955	19901011
	EP 495982	B1 199606	512	
	R: AT, BE,	CH, DE, DK, H	S, FR, GB, IT, LI, NL, SE	
	AT 139232	E 19960	AT 1990-914955	19901011
	ES 2087916	T3 199608	801 ES 1990-914955	19901011
	JP 2541702	B2 199610	009 JP 1990-513974	19901011
			.03 US 1992-839769	
PRAI	JP 1989-264763			
	WO 1990-JP1313			
os	MARPAT 115:71646			



- IT 134703-81-4P 135196-80-4P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, as drug for treatment of hypoxemia)
- RN 134703-81-4 CAPLUS
- CN Pyrido[2,3-d]pyrimidin-2-amine, 4-(5,6-dihydro-1(4H)-pyrimidinyl)-5,6,7,8-tetrahydro-N,8-di-2-propenyl- (9CI) (CA INDEX NAME)

$$H_2C = CH - CH_2 - NH$$

$$N$$

$$N$$

$$N$$

$$N$$

RN 135196-80-4 CAPLUS

CN Pyrido[2,3-d]pyrimidin-2-amine, 4-(5,6-dihydro-1(4H)-pyrimidinyl)-5,6,7,8-tetrahydro-N,8-di-2-propenyl-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 134703-81-4 CMF C17 H24 N6

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

L11 ANSWER 24 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1987:407208 CAPLUS

DN 107:7208

TI Pyrimidine derivatives having antiallergy, antiinflammatory, and immunosuppressant activity

IN Friary, Richard James; Siegel, Marvin Ira; Smith, Sidney Randal

PA Schering Corp., USA

SO PCT Int. Appl., 37 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN. CNT 1

					'N T T	CAM.
DATE	APPLICATION NO.	DATE	KIND	NO.	PATENT	
					-	
19860501	WO 1986-US899	19861106	A2	375	WO 8606	PI
		19870226	A 3	375	WO 8606	
		, JP, KR	FI, HU,	AU, DK,	W:	
	LU, NL, SE	, FR, GB, IT,	CH, DE,	AT, BE,	RW:	
19860501	AU 1986-58656	19861118	A 1	656	AU 8658	
19860501	EP 1986-903052	19870506	A1	82	EP 2202	
	LI, LU, NL, SE	, FR, GB, IT,	CH, DE,	AT, BE,	R:	
19860815	US 1986-897169	19880216	A	596	US 4725	
		19850501		729334	US 1985	PRAI
		19860501		-US899	WO 1986	
1986050	EP 1986-903052 LI, LU, NL, SE	19870506 , FR, GB, IT, 19880216 19850501	Al CH, DE,	82 AT, BE, 596 5-729334	EP 2202 R: US 4725 US 1985	PRAI

The title compds. [I; R = H, C1-6 alkyl, CH2CH2OH, CHO, acyl, (substituted) Bz or sulfonyl, carboxyalkyl, aminoalkyl; R1 = (substituted) Ph, pyridyl, furyl, thienyl, pyrrolyl, isoxazolyl, isothiazolyl, pyrazolyl; X = CH, CH2, N, NR; Y = O, S; Z = (CR2R3)m, (CR2:CR3)p; R2, R3 = H, alkyl; R2R3 = bond; m = 2-6; n = 0, 1; P = 1-3] were prepd. as allergy and inflammation inhibitors and as immunosuppressants. Thus, 2-chloronicotinoyl chloride was amidated with 2-(methylthio)-2-imidazoline-HI and the product cyclocondensed with PhNH2 to give pyridoimidazopyrimidinone II. In guinea pigs 2 mg II/kg orally inhibited anaphylactic bronchospasms.

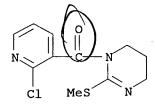
IT 108409-42-3P 108409-44-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and cyclocondensation of, with phenylamine deriv.)

RN 108409-42-3 CAPLUS

CN Pyrimidine, 1-[(2-chloro-3-pyridinyl)carbonyl]-1,4,5,6-tetrahydro-2-(methylthio)- (9CI) (CA INDEX NAME)





RN 108409-44-5 CAPLUS

CN Pyrimidine, 1-[(3-chloropyrazinyl)carbonyl]-1,4,5,6-tetrahydro-2-(methylthio)- (9CI) (CA INDEX NAME)

- L11 ANSWER 25 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
- AN 1987:28848 CAPLUS
- DN 106:28848
- Heterocyclic compounds TI
- Shiokawa, Kozo; Tsuboi, Shinichi; Kagabu, Shinzo; Moriya, Koichi IN
- Nihon Tokushu Noyaku Seizo K. K., Japan PA
- Eur. Pat. Appl., 271 pp. SO
 - CODEN: EPXXDW
- DTPatent
- LΑ German
- FF

LΑ		man							
FAN.	CNT								
	PAI	ENT NO.		KIND	DATE		AP.	PLICATION NO.	DATE
ΡI	EP	192060		A1	19860827		EP	1986-100708	19860117
		192060		B1	19910918			1300 100.00	1300011,
			BE.		, FR, GB,	IT.	LI.	VI.	
	JР	61178981	,	A2	19860811	,		1985-18627	19850204
		06006585		B4	19940126			2000 2002,	
		61178982		A2	19860811		JP	1985-18628	19850204
		06049699		B4	19940629			1300 10020	150001
		61183271		A2	19860815		JР	1985-23683	19850212
		07000613		B4	19950111		~ -	1500 1000	
		61267561		A2	19861127		JР	1985-106853	19850521
		06029258		В4	19940420				
		61267575		A2	19861127		JР	1985-106854	19850521
		05014716		B4	19930225				
		62081382		A2	19870414		JР	1985-219082	19851003
		07030070		В4	19950405				
		67493		E	19911015		AT	1986-100708	19860117
		4742060		Α	19880503		US	1986-821621	19860121
		8652866		A1	19860807			1986-52866	19860130
		584388		B2	19890525				
		77750		A 1	19891031		IL	1986-77750	19860131
		1276018		A1	19901106			1986-500793	19860131
	DK	8600519		Α	19860805			1986-519	19860203
		8600763		Α	19860924		ZA	1986-763	19860203
		8600428		Α	19861021			1986-428	19860203
	DD	242742		A 5	19870211		DD	1986-286723	19860203
	HU	41954		A2	19870629		HU	1986-466	19860203
	HU	200651		В	19900828				
	CS	255867		B2	19880315		CS	1986-754	19860203
	PL	149199		B1	19900131		PL	1986-257774	19860203
	HU	202365		В	19910328		HU	1989-5815	19860203
	ES	551629		A1	19871201		ES	1986-551629	19860204
	US	4845106		Α	19890704		US	1987-68991	19870701
	ES	557616		A1	19880216		ES	1987-557616	19870709
	ES	557617		A1	19880216		ES	1987-557617	19870709
		557618		A 1	19880216		ES	1987-557618	19870709
	US	5001138		Α	19910319		US	1989-347836	19890504
	US	5204360		Α	19930420		US	1990-557292	19900724
	US	5298507		Α	19940329		US	1992-832174	19920206
		05194490		A2	19930803		JP	1992-235152	19920812
		07020953		B4	19950308				
		9201042		Α	19920821		DK	1992-1042	19920821
		172809		B1	19990726				
		5461167		Α	19951024		US	1993-67642	19930525
		5428032		Α	19950627			1993-169902	19931220
	US	5580889		Α	19961203		US	1995-404849	19950315



	US	5750704	Α	19980512	US	1996-662096	19960612
	US	6022967	Α	20000208	US	1998-12620	19980123
	US	6297374	В1	20011002	US	1999-309988	19990511
PRAI	JP	1985-18627	Α.	19850204			
	JP	1985-18628	Α	19850204			
	JP	1985-23683	Α	19850212			
	JP	1985-106853	Α	19850521			
	JP	1985-106854	Α	19850521			
	JP	1985-219082	Α	19851003			
	ΕP	1986-100708	Α	19860117			
	US	1986-821621	A3	19860121			
	US	1987-68991	A3	19870701			
	US	1989-347836	A3	19890504			
	US	1990-557292	A3	19900724			*
	US	1992-832174	A3	19920206			
	US	1993-67642	A3	19930525			
	US	1993-169902	A3	19931220			
	US	1995-404849	A3	19950315			
	US	1996-662096	A3	19960612			
	US	1998-12620	A3	19980123			
OS	CAS	SREACT 106:2884	8				

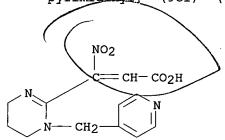
AΒ I (R, R1, R2, R5, R6 = H, alkyl; R3, R4 = H, OH, alkyl; n = 0, 1; X = 0, S, NR7, CHR8; Y = N, CR9; Z = 5- or 6-membered heterocyclic group; R7 = H, halo, OH, alkoxy, benzyloxy, alkyl, etc.; R8 = H, alkyl, aryl, benzyl; R9 = H, halo, OH, alkoxy etc.) were prepd. as insecticides. Thus, a mixt. of 4.3 g N-(2-chloro-5-pyridylmethyl)-3-aminopropanethiol and 4.3 g 1-nitro-2,2-bis(methylthio)ethylene in EtOH was refluxed for 10 h to give 1.3 g 3-(2-chloro-5-pyridylmethyl)-2-nitromethylenetetrahydro-2H-1,3thiazine (II). II, 200 ppm, totally controlled peach leaf louse (Myzodes persicae) on egg plant in the lab.

ΙT 105828-00-0P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of, as insecticide)

RN 105828-00-0 CAPLUS

2-Propenoic acid, 3-nitro-3-[1,4,5,6-tetrahydro-1-(4-pyridinylmethyl)-2-CN pyrimidinyl] - (9CI) (CA INDEX NAME)



- L11 ANSWER 26 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
- 1986:70362 CAPLUS AN
- DN 104:70362
- Poly(vinyl chloride) plastisols containing adhesion-promoting additives ΤI and their use as coatings
- Hurnik, Helmut; Groegler, Gerhard; Hess, Heinrich; Kopp, Richard IN
- Bayer A.-G. , Fed. Rep. Ger. Ger. Offen., 52 pp. PA
- SO

CODEN: GWXXBX

DTPatent

LΑ German

FAN.CNT 1

	PA'	ENT	NO.		KIN	ID	DATE			AP	PLICAT	ION NO.	DATE	
PI	DE	3403	 497		A]	 L	1985	0808		DE	1984-	3403497	19840	202
	EΡ	1508	03		A2	2	1985	0807		EP	1985-	100640	19850	123
	EΡ	1508	03		A3	3	1986	0212						
	EΡ	1508	03		в1	L	1988	0615						
		R:	AT,	BE,	CH,	DE	FR,	GB,	IT,	LI, I	NL, SE			
	ΑT	3514	4		E		1988	0715		AΤ	1985-1	100640	19850	123
	US	4623	686		Α		1986	1118		US	1985-	694562	19850	124
	CA	1255	042		A1	L	1989	0530		CA	1985-	472920	19850	125
	DK	8500	481		Α		1985	0803		DK	1985-	481	19850	201
	ZA	8500	792		Α		1985	0925		ZA	1985-	792	19850	201
	ES	5400	68		A1	L	1985	1116		ES	1985-	540068	19850	201
	JΡ	6018	8475		A2	2	1985	0925		.JP	1985-	17757	19850	202
PRAI	DE	1984	-3403	3497			1984	0202						
	ΕP	1985	-1006	640			1985	0123						

- AΒ The title compns. have good storage stability and contain PVC plastisols and finely divided polyisocyanates with retarded activity (i.e., prepd. by reaction of NCO groups with reactive compds.) as well as plasticizers and/or slightly branched, plastisol-compatible polyols m. <60.degree.. Thus, a suspension of 56 g monomer-free trimerized 2,4-TDI (polyisocyanurate with 15.5% NCO, particle size .apprx.10 .mu.) in 100 g DOP was mixed with 0.4 g 4,4'-methylenebis(2-methylcyclohexanamine) (I) to prep. a compn. which was stable even after the addn. of 17 g 2,4(or 6)-diamino-3,5-diethyltoluene at 40-60.degree. (without I, the suspension solidified in a few minutes). Adding 5.6 g of the I-contg. suspension to 100 g plastisol (1 kg PVC in 700 g DOP) gave a coating compn. which had a const. viscosity during >30 days (without I, the plastisol thickened after 1 day) and was applied to nylon 66 fabric to give a coating with adhesion 185 N/5 cm.
- $_{
 m IT}$ 83613-32-5D, reaction products with polyisocyanates RL: USES (Uses)

(adhesion promoter, PVC plastisol contq., stable)

- RN 83613-32-5 CAPLUS
- CN Pyrimidine, 1,1'-(1,2-ethanediyl)bis[1,4,5,6-tetrahydro-2-methyl-(9CI) (CA INDEX NAME)

Some 19

L11 ANSWER 27 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1982:598718 CAPLUS

DN 97:198718

TI Tetrahydropyrimidines and their use as catalysts in production of polyurethane plastics

IN Rasshofer, Werner; Groegler, Gerhard; Kopp, Richard

PA Bayer A.-G., Fed. Rep. Ger.

SO Eur. Pat. Appl., 72 pp.

CODEN: EPXXDW

DT Patent

LA German

ГАИ СИТ 1

PAN.	CNT I				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 54876	A1	19820630	EP 1981-110409	19811214
	R: BE, DE,	FR, GB	, IT, NL	•	
	DE 3049131	A 1	19820715	DE 1980-3049131	19801224
	JP 57130976	A2	19820813	JP 1981-206318	19811222
	US 4665177	Α	19870512	US 1985-762347	19850805
PRAI	DE 1980-3049131		19801224		
	EP 1981-110409		19811214		
	US 1981-332064		19811218		
	JP 1981-206318		19811222		

1,2-bis(tetrahydro-2-methylpyrimidin-1-yl)ethane [83613-32-5],
1,7-bis(tetrahydro-2-methylpyrimidin-1-yl)-4-methyl-4-azaheptane (I)
[83613-34-7], 1-[3-(dimethylamino)propyl]tetrahydro-2-methylpyrimidine
[83613-35-8] and several similar pyrimidine derivs. (as well as salts or complexes) are prepd. and used as catalysts for the prepn. of polyurethanes. The catalysts are resistant to hydrolysis and have little or no odor. Thus, [H2N(CH2)3NH(CH2)3]2NMe [83613-41-6] and MeCOCH2CO2Et [141-97-9] were used to prep. I. A mixt. of alkoxylated trimethylolpropane 80, HOCH2CH2OH 7, dibutyltin dilaurate 0.5, Cl3CF 12, I 0.4, and an isophorone diisocyanate-propoxylated glycerol prepolymer 41 g was used to prep. a polyurethane integral foam. The start time and cure time were 21 s and 122 s, resp.

IT 83613-32-5P 83613-36-9P 83613-37-0P

83613-39-2P 83613-40-5P

RL: PREP (Preparation)

(prepn. of and catalysis of polyurethane formation by)

RN 83613-32-5 CAPLUS

CN Pyrimidine, 1,1'-(1,2-ethanediyl)bis[1,4,5,6-tetrahydro-2-methyl- (9CI) (CA INDEX NAME)

RN 83613-36-9 CAPLUS

CN Carbonic acid, compd. with 1,1'-(1,2-ethanediyl)bis[1,4,5,6-tetrahydro-2-methylpyrimidine] (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 83613-32-5 CMF C12 H22 N4

CM 2

CRN 463-79-6 CMF C H2 O3

RN 83613-37-0 CAPLUS

CN Phenol, compd. with 1,1'-(1,2-ethanediyl)bis[1,4,5,6-tetrahydro-2-methylpyrimidine] (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 83613-32-5 CMF C12 H22 N4

CM 2

CRN 108-95-2 CMF C6 H6 O

RN 83613-39-2 CAPLUS

CN Hexanoic acid, 2-ethyl-, compd. with 1,1'-(1,2-ethanediyl)bis[1,4,5,6-tetrahydro-2-methylpyrimidine] (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 83613-32-5 CMF C12 H22 N4

CM 2

CRN 149-57-5 CMF C8 H16 O2

RN 83613-40-5 CAPLUS

CN Pyrimidine, 1,1'-(1,2-ethanediyl)bis[1,4,5,6-tetrahydro-2-methyl-, diacetate (9CI) (CA INDEX NAME)

CM 1

CRN 83613-32-5 CMF C12 H22 N4

CM 2

CRN 64-19-7 CMF C2 H4 O2

L11 ANSWER 28 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1982:142520 CAPLUS

DN 96:142520

Studies on .beta.-lactams. Part 59. A convenient synthesis of TΤ .alpha.-amido-.beta.-lactams

Bose, Ajay K.; Manhas, M. S.; Van der Veen, J. M.; Amin, S. G.; Fernandez, ΑU I. F.; Gala, K.; Gruska, R.; Kapur, J. C.; Khajavi, M. S.; et al.

Dep. Chem. Chem. Eng., Stevens Inst. Technol., Hoboken, NJ, 07030, USA CS

SO Tetrahedron (1981), 37(13), 2321-34 CODEN: TETRAB; ISSN: 0040-4020

DTJournal

LA English

AB A method is described for the prepn. of a no. of .alpha.-amido-.beta.lactams starting from an azomethine and H2NCH2CO2H, protected as a Dane salt by reaction with a .beta.-dicarbonyl compd. Stereospecific condensation reaction between the Dane salts and imines or thioimidates gave 40-60% (.beta.-carbonylvinylamino)-2-azetidinones. E.g., reaction of Et02CCH: CMeNHCH2CO2- K+ with a methoxyphenyldihydroisoguinoline (Et3N, -25.degree.) gave 80% I, the structure of which was detd. by x-ray crystallog. anal. Mild acid hydrolysis of the vinylamino side chains followed by acylation gave the title compds. Isotope-labeled .beta.-lactams and intermediates for some .beta.-lactam antibiotics were prepd. by this method.

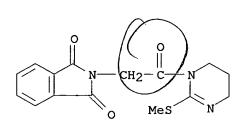
IT 54679-27-5P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(condensation reaction of, with Dane salt in .alpha.-amido-.beta.lactam prepn., stereospecific)

RN

54679-27-5 CAPLUS
Pyrimidine, 1-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)acetyl]-1,4,5,6-CN tetrahydro-2-(methylthio)- (9CI) (CA INDEX NAME)



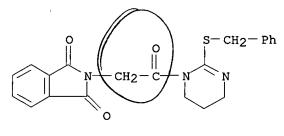


- L11 ANSWER 29 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN
- AN 1975:140071 CAPLUS
- DN 82:140071
- TI Synthesis of exocyclic thioanalogs of azacepham
- AU Bose, Ajay K.; Kapur, J. C.; Manhas, M. S.
- CS Dep. Chem. Chem. Eng., Stevens Inst. Technol., Hoboken, NJ, USA
- SO Synthesis (1974), (12), 891-4 CODEN: SYNTBF; ISSN: 0039-7881
- DT Journal
- LA English
- AZacephams I (R = CO2Et, COCH2Ph, phthalimidoacetyl; R1 = SMe, SCH2Ph; R2 = OPh, phthalimidoacetyl, OCH2Ph, OMe, N3) were prepd. by treating tetrahydropyrimidines II (R = H, R1 = SMe, SCH2Ph) with the acyl chloride and treating II (R = CO2Et, COCH2Ph, phthalimidoacetyl; R1 = SMe, SCH2Ph) with R2CH2COCl. I (R = COCH2OPh, R1 = SMe, R2 = OPh) was obtained in 1 step from II (R = H, R1 = SMe) and PhOCH2COCl. Redn. of I (R = phthalimidoacetyl, R1 = SMe, R2 = N3) and acylation gave I (R = phthalimidoacetyl, R1 = SMe, R2 = NHCOCH2OPh). Oxidn. of I (R = COCH2Ph, R1 = SMe, R2 = OPh) yielded I (R = COCH2Ph, R1 = OH, R2 = OPh).
- IT 54679-26-4P 54679-27-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

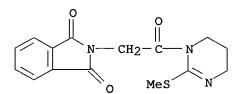
(prepn. and reaction of, with substituted acetyl chlorides)

- RN 54679-26-4 CAPLUS
- CN Pyrimidine, 1-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)acetyl]-1,4,5,6-tetrahydro-2-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)



RN 54679-27-5 CAPLUS

CN Pyrimidine, 1-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)acetyl]-1,4,5,6-tetrahydro-2-(methylthio)- (9CI) (CA INDEX NAME)



L11 ANSWER 30 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1974:132361 CAPLUS

DN 80:132361

TI Polyfluoroheterocyclic compounds. XXIII. Monoenes and dienes derived by the fluorination of hexafluorobenzene and of perfluoro and chlorofluoro heteroaromatic compounds. Mechanism for fluorination by cobalt fluorides

AU Chambers, Richard D.; Clark, David T.; Holmes, Thomas F.; Musgrave, W. Kenneth R.; Ritchie, Ian

CS Chem. Dep., Univ. Durham, Durham, UK

SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1974), (1), 114-25 CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

LA English

AB C6F6 with CoF3 and CaF2 gave perfluoro-1,4-cyclohexadiene and -cyclohexene. Similarly chlorofluoropyridines gave perhalodi- and -tetrahydropyridines and small amts. of acylic azaalkenes.

Tetrafluoropyrazine gave 5,6-dihydrohexafluoropyrazine. Calcns. of charge and spin ds. on the atoms in the ring at various stages in the fluorination were made and a mechanism involving, at each stage, the quenching of the first formed radical cation by F- and then by F was suggested. The formation of perfluoro-1,1'-bi-1,3-diazacyclohex-2-enyl from tetrafluoropyrimidine supported the mechanism.

IT 52126-62-2P

RN 52126-62-2 CAPLUS

CN 1,1'(4H,4'H)-Bipyrimidine, 2,2',4,4,4',4',5,5,5',5',6',6,6',6'-tetradecafluoro-5,5',6,6'-tetrahydro-(9CI) (CA INDEX NAME)



L11 ANSWER 31 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

1973:97631 CAPLUS AN

DN 78:97631

TI Thiazole derivatives

Tchelitcheff, Serge IN

Societe des Usines Chimiques Rhone-Poulenc PA

SO Fr. Demande, 9 pp. CODEN: FRXXBL

DT Patent

French LΑ

FAN. CNT 1

	U.1. 1				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2128071	A 5	19721020	FR 1971-7287	19710303
	FR 2128071	B1	19740802		
PRAT	FR 1971-7287		19710303		

Imidazolinylthiazoles (I, R = Me, Et, Hexyl, PhCH2, 2-pyridylmethyl) were prepd. from 2-bromo-5-nitrothiazole and 2-alkylthio-2-imidazolines. Antibiotic activity data were given for I.

IT40689-09-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN

40689-09-6 CAPLUS
Pyrimidine, 1,4,5,6-tetrahydro-2-(methylthio)-1-(5-nitro-2-thiazolyl)-CN (9CI) (CA INDEX NAME)



L11 ANSWER 32 OF 34 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1971:22905 CAPLUS

DN 74:22905

Antiinflammatory alkylthioimidazolines, tetrahydropyrimidines, and ΤI tetrahydrodiazepines

IN Eberle, Marcel K.

PA Sandoz Inc.

U.S., 3 pp. SO CODEN: USXXAM

DT Patent

English LΑ

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI US 3536714	Α	19701027	US 1967-679635	19671101	
PRAT US 1967-679635		19671101			

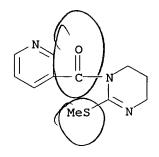
AΒ The title compds., I, useful as antiinflammatory agents were prepd. by acylation of the appropriate amine. I prepd. were (R and X given): Ph, CH2CH2; o-BrC6H4, CH2CH2; 3-pyridyl, CH2CH2; 4-pyridyl, CH2CH2; 2-(p-chlorobenzoyl)phenyl, CH2CH2; 2-pyridyl, 104.degree.; pyridyl (CH2)3.

30156-32-2P IT

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN

30156-32-2 CAPLUS
Pyrimidine, 1,4,5,6-tetrahydro-2-(methylthio)-1-nicotinoyl- (8CI) CN INDEX NAME)





=> d his

(FILE 'HOME' ENTERED AT 08:27:19 ON 15 DEC 2003)

FILE 'REGISTRY' ENTERED AT 08:27:25 ON 15 DEC 2003 L1SCREEN 1839 L2 SCREEN 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047 L3 STRUCTURE UPLOADED L4QUE L3 AND L1 NOT L2 L5 SCREEN 1839 SCREEN 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047 L6 L7 STRUCTURE UPLOADED QUE L7 AND L5 NOT L6 rs1 S L8 SSS SAM L9 L10 71 S L8 SSS FUL

FILE 'CAPLUS' ENTERED AT 08:29:53 ON 15 DEC 2003 L11 34 S L10

FILE 'CAOLD' ENTERED AT 08:30:43 ON 15 DEC 2003

=> s 110

L12 1 L10

=> d 112 bib, hitstr

L12 ANSWER 1 OF 1 CAOLD COPYRIGHT 2003 ACS on STN

AN CA57:16568b CAOLD

TI xanthene and thiaxanthene cyclic amidines

AU Faust, John A.; Sahyun, M.

DT Patent

TI xanthene and thiaxanthene cyclic amidines

AU Sahyun, Melville

DT Patent

ΡI

Laccine		
PATENT NO.	KIND	DATE
US 3042674		1962

IT 98470-57-6

RN 98470-57-6 CAOLD

CN Pyrimidine, 1,4,5,6-tetrahydro-1-(thioxanthen-9-ylmethyl)-, hydrochloride (7CI) (CA INDEX NAME)

Same M# 34 ^

● HCl